Statistical Mechanics 2012/2013 Problem Set 1

Submission date: 19.11.12

1.1 Two level system with degeneracy (30 points)

Consider a system of N distinguishable particles, in which the energy of each particle can assume one of two distinct values, 0 or ϵ (with $\epsilon > 0$). The higher energy level has a g-fold degeneracy. The total energy in the system is E. Assume $N, E \gg 1$.

(a) Find the entropy of the system.

(b) Find the temperature as a function of E, and show that it can be negative. What happens when a system of negative temperature is allowed to exchange heat with a system of positive temperature?

(c) Express the occupation number of the lower energy state in terms of the temperature and compare it to the probability of the lower energy state as calculated in the canonical ensemble.

(d) Consider for example a system with $E = 3N\epsilon/4$ in contact with a heat bath at temperature $T = 500K$, with $g = 2$. In what direction does the heat flow?

(e) The original system (uncoupled from a heat bath) is brought into contact with a similar system (with the same N, E and ϵ), whereby the two systems can exchange both energy and particles. In the second system both energy levels are non-degenerate. Obtain the change in the total entropy of the two systems before and after they were brought together by considering the combined system within the microcanonical ensemble. Is this a reversible process?

1.2 Ensemble equivalence and the Laplace method (30 points)

Consider a spin-1 model composed of a one dimensional chain of L spins subjected to a magnetic field, h. The energy of the spin is given by

$$E = hM = h\sum_{i=1}^{N} \sigma_i, \tag{1}$$

where $\sigma_i = +1, -1$ or 0.

(a) Calculate the leading order term in L of $S(E) = k_B \ln[\Omega(E)]$ in the micro-canonical ensemble using *using the Laplace method*. To this end you first have to estimate the partition sum by the appropriate integral and then evaluate it using the Laplace method. How does the next to leading coorection term in $S(E)$ scale with L ? What is the average number of 0 spins , $\langle N_0 \rangle = \langle \sum_{i=1}^{N} (1 - \sigma_i^2) \rangle$?

* 2 bonus points will be given for students who succeed in computing $\Omega(E)$ exactly, *in addition to using the Laplace method.*

(b) Calculate exactly $Z(\beta)$ in the canonical ensemble *without using the Laplace method.* As you can see, moving to a 'higher ensemble' may allow one to calculate the exact partition function more easily. Compute $\langle N_0 \rangle$ in the canonical ensemble as a function of L and $\langle E \rangle$. Did you obtain the same results as in (a) ?

* In principle, if we wanted to show that the two ensembles are equivalent we should have compared the free energy as obtained in both cases, and shown that they are equal up to corrections that scale as $\log L$. Unfortunately, this calculation is a rather involved.

1.3 Monte Carlo simulation (40 points)

In this question you will examine the central limit theorem in a two-dimensional Ising model with Metropolis dynamics. Note that although the Metropolis dynamics is probably not a realistic model of the dynamics of real magnets (as was stressed in class), it is nonetheless instructive from a theoretical perspective to explore this dynamics.

Consider a two dimensional Ising model on an $L \times L$ square lattice with periodic boundary conditions. The Hamiltonian of the model is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{2}$$

where $s_i = \pm 1$ and $\sum_{\langle i,j \rangle}$ denotes a sum over all nearest neighbour pairs. This model undergoes a phase transition at $T_c = 2J/\log(1+\sqrt{2}) \simeq 2.27J$. In this question, set $T = 3J$ to assure that the system is in the disordered phase.

Implement the metropolis algorithm in your favorite programming language. Work with the largest system for which you can collect enough statistics. In C, Fortran, Java and similar languages you should be able to reach systems of size $L = 200$, while in Matlab you will probably be limited to $L \approx 10$. Therefore, it is preferable that you do not run the simulation in Matlab if possible. You may download from the course website a code example written in C++, which you may alter to model the Ising dynamics. This code can be easily compiled on the computers found in the computer lab, as explained in the instructions attached to it.

(a) Verify that you are in the disordered phase by measuring that $\langle M \rangle = \langle \sum_i s_i \rangle = 0$ at $T = 3J$. Attach a plot of $M(t)$.

(b) Measure the correlation function for the magnetization

$$C(\Delta t) = \langle (M(t) - \langle M \rangle)(M(t+\Delta t) - \langle M \rangle) \rangle, \tag{3}$$

for several values of Δt. Estimate $\tau_{\rm relax}$ from $C(\Delta t)$ and attach a plot of $C(\Delta t)$.

(c) Measure the fluctuations in the magnetization by averaging

$$\sigma_M^2 = \left\langle (M - \langle M \rangle)^2 \right\rangle \tag{4}$$

at time steps larger than $\tau_{\rm relax}$. Measure the fluctuations for several system sizes (smaller than the maximal one you can simulate) and plot a graph which demonstrate that σ_M scales with L as you would expect from the central limit theorem.

Note: Please attach your code to your answer. You may work in pairs, but everyone should write his/her own code and produce his/her own plots. Also, make sure to save your code, as it will be useful for future homework assignments.